

Nonane  
111-84-2 | DTXSID9025796

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $8.45\text{e-}12\text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Inside

**Local applicability domain index:**  $8.29\text{e-}01$

**Confidence level:**  $8.98\text{e-}01$

## Nearest Neighbors from the Training Set

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Nonane

**Measured:**  $1.02\text{e-}11$

**Predicted:**  $8.45\text{e-}12$

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Decane

**Measured:**  $1.16\text{e-}11$

**Predicted:**  $1.10\text{e-}11$

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Octane

**Measured:**  $8.68\text{e-}12$

**Predicted:**  $7.74\text{e-}12$

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Hexane, 2,2-dimethyl-

**Measured:**  $4.83\text{e-}12$

**Predicted:**  $5.67\text{e-}12$

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2,4-Dimethylpentane

**Measured:**  $5.16\text{e-}12$

**Predicted:**  $5.28\text{e-}12$